SUBJECT: PRODUCT CHEMISTRY REVIEW – Antimicrobials Division
DP Barcode D242885 Reg. No. or File Symbol 3377-38
Manufacturing-Use [✓] OR End-Use Product [ ]

TO: Velma Noble/Tracy Lantz
PM Team No. 31

FROM: Anna Skapars, Chemist
Efficacy and Science Support Branch

THRU: Michelle Wingfield, Acting Chief
Efficacy and Science Support Branch

SUMMARY OF INFORMATION REVIEWED AND FINDINGS

Provided product chemistry data in MRID Nos: 444674-01, 444674-02, 444674-03 provides data for Guideline Series 61, 62 and 63.
These data are in compliance with 40 CFR part 158.155 through 158.190 and it satisfies product chemistry data for this product for reregistration.

Confidential Statement of Formula dated 1-6-98 is not filled out correctly and it does not comply with PR Notice 91-2 and it should be revised.
Registrant may not repackage the same product under the same EPA Reg. No.

Submit revised Confidential Statement of Formula and list all ingredients in the formula including the amount, the percent by weight and the limits for each ingredient in the formula.

Revise the lower limit for the active ingredient which should be lower than 80% which is the nominal concentration.

Ask them to calculate using table in 40 CFR.

Anna Skapars
7-2-98

TABLE 1: SUMMARY OF PRODUCT CHEMISTRY DATA REQUIREMENTS

EPA Reg. No. 3377-38

GLR #	TITLES		
	Series 61-Product Identity and Composition (40CFR§158.155, 160, 162, 165 & 167)		
61-1	Product Identity & Disclosure of Ingredients	A	444674-01
61-2	Description of Starting Materials & Manufacturing Process	A	444674-01
61-3	Discussion of Formation of Impurities	A	444674-01
	Series 62-Analysis and Certification of Product Ingredients (40CFR§158.170, 175 & 180)		
62-1	Preliminary Analysis of Product Samples	A	444674-02
62-2	Certification of Ingredient Limits		
62-3	Analytical Methods to Verify Certified Limits	A	444674-02
	Series 63-Physical and Chemical Characteristics (40CFR§158.190)		
63-2	Color	A	444674-03
63-3	Physical State	A	
63-4	Odor	A	
63-5	Melting Point	N/A	
63-6	Boiling Point	W	
63-7	Density, Bulk Density, or Specific Gravity	A	
63-8	Solubility	A	
63-9	Vapor Pressure	W	
63-10	Dissociation Constant	W	
63-11	Octanol/Water Partition Coefficient	N/A	
63-12	pH	A	
63-13	Stability	A	
63-14	Oxidizing or Reducing Action	N/A	
63-15	Flammability	A	
63-16	Explodability	A	
63-17	Storage stability	A	
63-18	Viscosity	A	
63-19	Miscibility	N/A	
63-20	Corrosion Characteristics	A	
63-21	Dielectric Breakdown Voltage	N/A	

A - Acceptable
W - Waived
NA - Not Applicable
DG - Data Gap

Reviewer: Anna Skapars

Section Head _____

Date: _____

ALKYL DIMETHYL BENZYL AMMONIUM CHLORIDE

Shaughnessy No. 069104

(DP Barcode D242885)

Antimicrobial Division: Product Chemistry Review

April 22, 1998

Contract No. 68-D4-0010

Submitted to:
U.S. Environmental Protection Agency
Arlington, VA

Submitted by:
Dynamac Corporation
The Dynamac Building
2275 Research Boulevard
Rockville, MD 20850-3268

REVIEW OF PRODUCT CHEMISTRY, OPPTS 830 SERIES

Chemical Name (IUPAC, ANSI, etc.)	Alkyl* dimethyl benzyl ammonium chloride *(60% C_{14}, 30% C_{16}, 5% C_{18}, 5% C_{12}); ADBAC
Chemical Number (CAS; PC Code)	CAS No. 68391-01-5 PC Code 069104
Product Name	Albemarle BQ1416-8 Biocide
EPA Reg. No.	3377-38
Type of Product (T, FI, MP, EP)	80% FI
DP Barcode	D242885
Submission No.	S536945
Case No. / Type	061919 / Registration
Reviewer	
Approvals	
Section/Team	
Branch Senior Scientist	
Branch Chief	

INTRODUCTION

Albemarle Corporation has submitted product chemistry data (1998; MRIDs 44467401-44467403), a CSF dated 1/6/98, and a specimen product label for the 80% alkyl dimethyl benzyl ammonium chloride (ADBAC) formulation intermediate; the 80% FI is a quaternary ammonium salt product produced by an integrated system. Albemarle Corporation (formerly Ethyl Corporation) is a member of the ADBAC QUAT Joint Venture and is considered to be the original data submitter for all data submitted by Ethyl Corporation.

CONCLUSIONS

OPPTS 830.1550 Product Identity and Composition and OPPTS 830.1750 Certified Limits

1. The submitted information and CSF are not adequate. A revised CSF including nominal concentrations and upper and lower certified limits for the active and inert ingredients and nominal concentrations and upper certified limits for impurities present at ≥0.1% must be submitted on EPA Form 8570-4 along with explanations of how certified limits were established. In addition, the label claim of 80% reflects the proposed lower certified limit rather than the nominal concentration of the active ingredient, as required in PR Notice 91-2, and must be revised.

OPPTS 830.1600 Description of Materials Used to Produce the Product
OPPTS 830.1650 Description of Formulation Process
OPPTS 830.1700 Preliminary Analysis

2. The submitted information concerning the starting materials and formulation process and preliminary analysis is adequate.

OPPTS 830.1670 Discussion of Formation of Impurities

3. The submitted discussion of formation of impurities is not adequate. Additional discussion concerning the potential for formation of nitrosamines and post-production impurities must be submitted.

OPPTS 830.6302-830.7950 Physical/Chemical Properties

4a. AD has no objections to granting the data waivers requested for boiling point, dissociation constant, and vapor pressure (OPPTS 830.7220, 830.7370, and 830.7950).

4b. Adequate data have been submitted concerning most of the remaining physical/chemical properties of the 80% FI and practical equivalent of the TGAI except that additional data are required for storage stability and solubility (OPPTS 830.6317 and 830.7840-830.7860) and data pertaining to UV/visible absorption (OPPTS 830.7050) remain outstanding. Quantitative data must be submitted reflecting the stability of the FI stored in the typical storage container under ambient conditions for at least one year, and data reflecting the solubility of the practical equivalent of the TGAI in organic solvents must be submitted.

DETAILED CONSIDERATIONS

Group A--Product Identity, Composition, and Analysis

OPPTS 830.1550 Product Identity and Composition and OPPTS 830.1750 Certified Limits

Albemarle Corporation submitted information (MRID 44467401) and a CSF dated 1/6/98 for the 80% ADBAC FI which are presented in Confidential Appendix A.

OPPTS 830.1600 Description of Materials Used to Produce the Product

OPPTS 830.1620 Description of Production Process

The registrant submitted (MRID 44467401) the source, material specifications/material safety data sheets, and relative amounts of the starting materials, along with a complete description of the batch manufacturing process including the manufacturing equipment, temperature and quality control requirements.

OPPTS 830.1670 Discussion of Formation of Impurities

The registrant submitted (MRID 44467401) a discussion of formation of impurities addressing impurities resulting from carrryover of unreacted starting materials or impurities of the starting materials and impurities resulting from side reactions. The registrant did not include discussion of the potential for formation of nitrosamines or post-production impurities.

OPPTS 830.1700 Preliminary Analysis

The registrant submitted (MRID 44467402) results of preliminary analysis of five batches of the 80% ADBAC FI which are presented in Confidential Appendix A.

Group B--Physical/Chemical Properties

The registrant submitted (MRID 44467403) physical/chemical data for the 80% ADBAC FI. Data waivers were requested for boiling point, dissociation constant, and vapor pressure (OPPTS 830.7220, 830.7370, and 830.7950) as detailed below.

Table 1. Physical/chemical properties of the 80% ADBAC FI.

Guideline Number	Property	**Description** [Method]
830.6302	Color	**APHA color 50**
830.6303	Physical State	**Liquid**
830.6304	Odor	**Ethanolic**
830.6313	Stability	**Stable for 14 days at 55 C and when exposed to light, high density polyethylene (HDPE) at 55C, and stainless steel at ambient conditions and at 55 C** [NMR/titration quantitation]
830.6314	Oxidation/Reduction	**N/A; does not contain oxidizing or reducing agents**
830.6315	Flammability	**37.0 C** [Tag Closed Flash Tester]
830.6316	Explodability	**N/A; does not contain any components subject to explosion and is packaged in a non-pressurized container**
830.6317	Storage Stability	**Stable for 30 days stored in HDPE at 55 C** [NMR/titration quantitation]
830.6319	Miscibility	**N/A; is not an emulsified liquid and is to be diluted only with water**
830.6320	Corrosion Characteristics	**HDPE - no noticeable color change, and less than 3% change in weight, dimension, volume, and hardness following 7 days exposure at 55 C Stainless steel - 0.3 mpy average corrosion rate at 55 C with broad shallow pitting evident; 0.2 mpy average corrosion rate under ambient conditions with some shallow pitting**
830.7000	pH	**7.59; 10% solution**
830.7050	UV/Visible Absorption	Not reported
830.7100	Viscosity	**507.0 cSt at 25 C** [viscometer]
830.7200	Melting Point/Melting Range	**N/A; FI is a liquid**
830.7220	Boiling Point/Boiling Range	**Waiver requested; FI is a multicomponent system with different boiling points for each component, therefore a stable and meaningful boiling point cannot be obtained**

Guideline Number	Property	**Description** [Method]
830.7300	Density/Relative Density/Bulk Density	**Specific gravity 0.9429 at 25 C** [Parr Density Meter]
830.7370	Dissociation Constant in Water	**Waiver requested; FI contains water and is already dissociated to some extent**
830.7550 830.7560 830.7570	Partition Coefficient (Octanol/Water)	**N/A; FI is not an organic nonpolar substance**
830.7840 830.7860	Solubility	**Completely soluble in water**
830.7950	Vapor Pressure	**Waiver requested; quaternary ammonium chloride does not azeotrope with water, therefore any vapor pressure measured would be that of water**

Attachment: Confidential Appendix A

Inert ingredient information may be entitled to confidential treatment

Manufacturing process information may be entitled to confidential treatment

CONFIDENTIAL APPENDIX A (DP Barcode D242885)

[redacted]

The submitted data are adequate.

Manufacturing process information may be entitled to confidential treatment

Inert ingredient information may be entitled to confidential treatment